

## LA-UR-19-28561

Approved for public release; distribution is unlimited.

Title: xRage: Setting ambient region state

Author(s): Menikoff, Ralph

Intended for: LANL seminar

Issued: 2019-08-23

---

**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

# xRage: Setting ambient region state



**Ralph Menikoff, T-1**

August, 2019

Acknowledgement: John Grove



Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

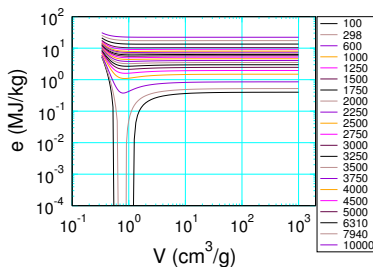
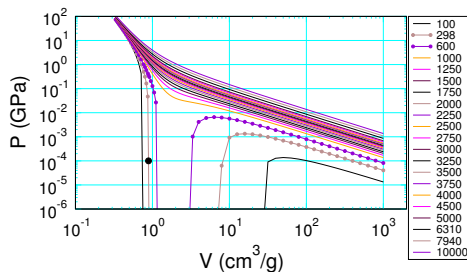
# Sesame table

Equation of state (EOS)

Independent thermodynamic variables:  $\rho$  and  $T$

Tables for  $P(\rho, T)$  and  $e(\rho, T)$

Example: Nitromethane isotherms (log-log scale to cover wide domain)

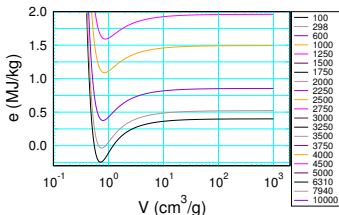
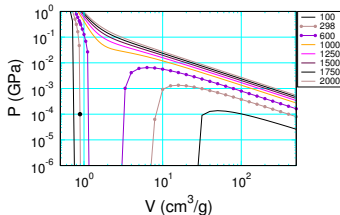
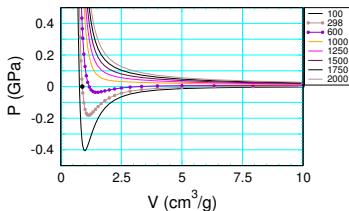


Phase space of interest for detonation wave simulation  $P > 0.1$  GPa

Issue at ambient state: 1 bar and 298 K, despite point in table

# van der Waal loop

Compressibility  $K_T = -V(\partial_V P)_T > 0$  required for thermodynamic stability  
 $K_S = K_T + \Gamma^2(C_V T/V) > 0$  required for thermodynamic consistency  
required for hydro PDEs to be hyperbolic (non-linear wave equations)



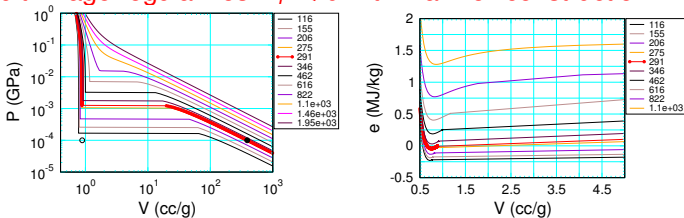
# Maxwell construction and mixed region

xRage generates teos table:  $P$ ,  $T$  independent variables

Facilitates PT equilibrium for mixed cell (default hydro)

Unique PT solution only if component EOS are consistent & stable

By default xRage regularizes  $K_T < 0$  with Maxwell construction



Horizontal lines in  $P$  plot define **mixed liquid-vapor region**

Small liquid drops surrounded by vapor or phase separated liquid & vapor

**Initialization issue**

$T=298$  K isotherm has  $P \approx 10^{-3}$  GPa or 10 bar

EOS density at ambient state,  $\rho < 0.01$  g/cc (**vapor region**)

**Liquid NM at ambient state** has  $\rho = 1.125$  g/cc

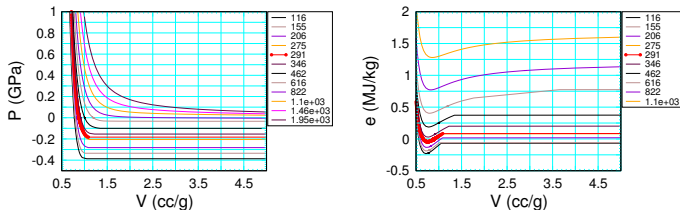
# Comments on EOS

- Even though ambient density not as intended  
Not coding error
- Issue is with nitromethane table  
Peak pressure on van der Waal loop is too high  
With Maxwell construction EOS is qualitatively correct  
But quantitatively inaccurate at low pressures  
High pressure regime not affected by Maxwell construction
- Limited data to calibrate EOS  
Data for shock compression  
Fitting form extrapolated to expansion  
Extrapolations can be quantitatively inaccurate

# Work around

`support_tension = .true.`

Instead of Maxwell construction,  
isotherm extended at minimum pressure on van der Waal loop



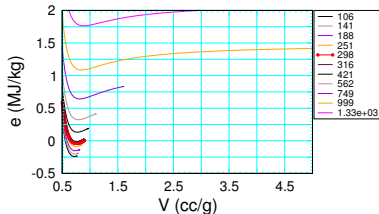
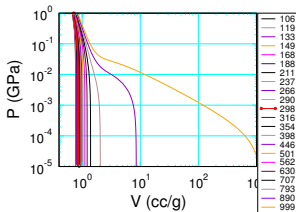
Next issue:

Nearest isotherm to 298 K room temperature is  $T = 291$  K  
Interpolated density slightly off (depends on teos grid spacing)  
even though sesame table has isotherm at 298 K



# Adjust teos grid

Set teos.in input `tevlo`, `tevhi`, `numtevdec` such that  
 $\text{tevlo} = T0 * 10^{(-j/\text{numtevdec})}$  for some integer  $j$   
and similarly for  $P0$



Then for xRage input

$\text{tevreg}=T0$  and  $\text{prsreg}=P0$

get value of density from point on sesame table

# Comment on interpolation

- **Sesame table to teos table**

Independent variables  $(V, T) \leftrightarrow (P, T)$

1 to 1 iff  $P(V)$  monotonic on all isotherms ( $K_T > 0$ )

In mixed region  $P$  is constant on isotherm and  $V$  not unique

Mixed cell EOS equations ( $P$ - $T$  equilibrium) can be stiff

- **Accuracy of interpolation**

Depends on smoothness of function relative to  $(P, T)$  grid

Logarithmic grid spacing increases accuracy for large  $P$   
but not helpful in mixed region with support tension

`numprsddec`, `numtevdec` sets grid size

but accuracy can be limited by coarse grid on sesame table

- **Derivatives** (such as sound speed)

On grid lines, normal derivative is discontinuous